Revision 1.2, October 7, 2010, Instructor: Jochen Autschbach

General

NMR parameters et al.
Electronic absorption and electronic optical activity
Photochemistry: Absorption, emission, energy transfer

This course is subdivided into three 'Mini Courses', i.e. three 5–week units that may be taken as a whole 3–credit course, or as independent 1–credit units.

The topic of the first 5–week course segment is the theoretical foundation of frequency–independent spectroscopic properties of molecules. You will also perform practical computations. The main focus will be on computing *NMR parameters* such as chemical shifts and nuclear spin–spin coupling constants. As an example, we will work out how C–H coupling constants relate to the hybridization of the carbon atoms. You will find out that one can actually measure the hybridization by NMR! If time permits, we will take a quick look at molecular EPR parameters.

In the second 5–week unit we will discuss the theory underlying computations of *time– or frequency–dependent properties* of molecules. With this formalism, it is possible to treat important properties such as electronic absorption and the dynamic molecular polarizability, as well as circular dichroism and optical rotation for chiral molecules. As in the other course units, this section offers practical experience with time–dependent density functional (TD–DFT) calculations of absorption and CD spectra of small molecules.

The third 5–week unit deals more generally with photochemistry. Topics are: electronic absorption, emission (fluorescence, phosphorescence), classical description of absorption processes, quantum theory of absorption, quantum yield, Einstein coefficients, energy transfer (Foerster mechanism, collisions), intersystem crossing, solvent effects, selection rules. We will attempt calculations of the wavelength shift between absorption and emission for a small molecule.

Time, Dates, Location, Office Hours, Contact Info

Class Room: 106 Baldy
Lecture Times: T R, 0930 – 1050
Office Hours: Monday 5:00 – 6:00 pm, NSC Room 313
Instructor email: jochena@buffalo.edu
Phone: 645-4122

Textbook

There is no mandatory textbook for this unit. Recommended textbooks that cover the calculation of molecular spectroscopic properties are

1. Ira N. Levine, *Quantum Chemistry*, Prentice Hall
2. Peter W. Atkins, *Molecular Quantum Mechanics*, Oxford University Press

as well as Atkins' standard physical chemistry textbook and most other undergraduate PChem texts. There are no reading assignments for which you would need a specific textbook.

Course Web Site

A web site for the course will be available at UB–Learns (https://ublearns.buffalo.edu) after the first day of class. I will post there copies of the assignments, additional course information, copies of the handouts, and important notices.

Grading, etc.

Each unit's grade will be based on a homework assignment (paper & pencil calculations, and computations of spectral parameters using quantum chemistry software (Gaussian, ADF), 50%) and a 1-hour exam at the end of each 5–week unit (50%).